

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 7.00e-11 mmHg

Global applicability domain: Outside

Local applicability domain index: 2.56e-01

Confidence level: 2.73e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Lepidine</div> <div>Measured: 8.02e-14</div> <div>Predicted: 9.90e-03</div>	<div>Image not found</div> <div>Perflutren</div> <div>Measured: 1.66e-08</div> <div>Predicted: 7890</div>	<div>Image not found</div> <div>2,2,5,5-Tetramethylhexane</div> <div>Measured: 9.80e-08</div> <div>Predicted: 7.94</div>
<div>Image not found</div> <div>Benz(a)anthracene</div> <div>Measured: 1.97e-10</div> <div>Predicted: 2.14e-08</div>	<div>Image not found</div> <div>4-Chloro-3-methylphenol</div> <div>Measured: 1.50e-12</div> <div>Predicted: 5.35e-02</div>	